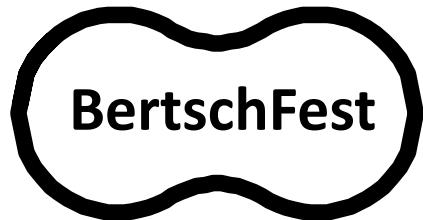
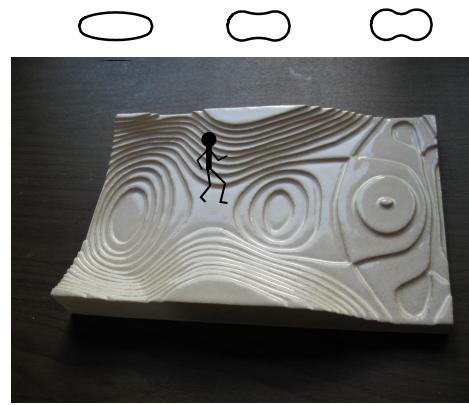


Symposium on the occasion of George Bertsch's 70th birthday

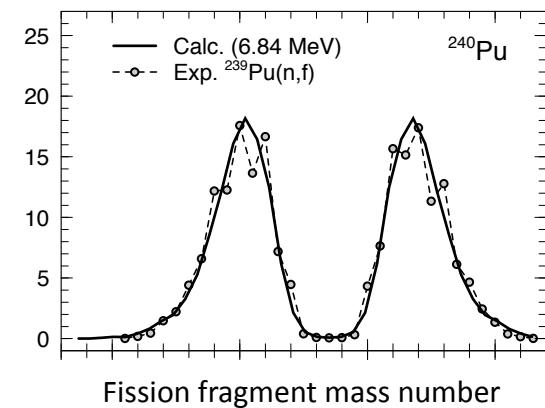


Nuclear shape dynamics

Jørgen Randrup, LBNL
Berkeley, California



Nuclear deformation energy

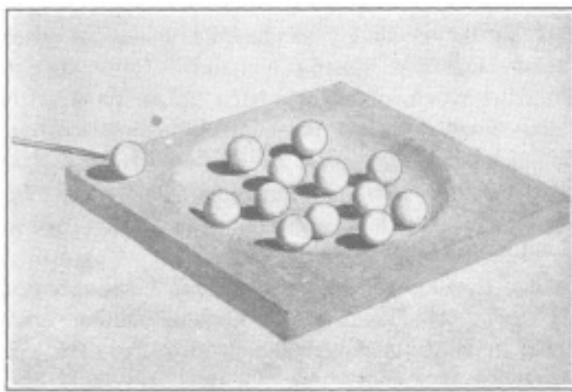


Basic concepts in nuclear fission

Compound nucleus

Nature 137 (1936) 351 quoting Niels Bohr:

“.. the energy of the incident neutron will be rapidly divided among all the nuclear particles ..”



Niels Bohr, *Nature* 137 (1936) 344:

“.. neutron capture .. will result in .. the formation of a compound system of remarkable stability. The possible later breaking up of this system .. must in fact be considered as separate competing processes which have no immediate connexion with the first stage ..”

Niels Bohr, *Nature* 143 (1939) 330:

“.. any nuclear reaction initiated by collisions or radiation involves as an intermediate stage the formation of a compound nucleus in which the excitation energy is distributed among the various degrees of freedom in a way resembling thermal agitation ..”

Shape evolution

N. Bohr & J.A. Wheeler, *Phys Rev* 56 (1939) 426:

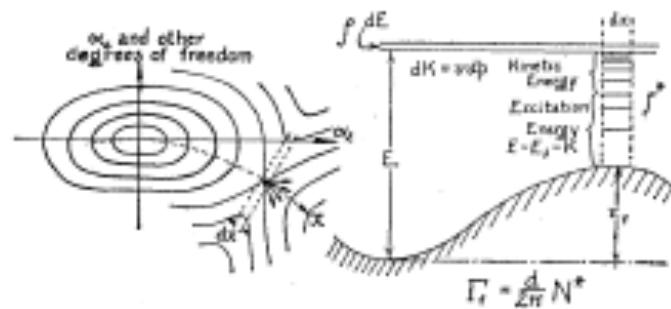


FIG. 3. The potential energy associated with any arbitrary deformation of the nuclear form may be plotted as a function of the parameters which specify the deformation, thus giving a contour surface which is represented schematically in the left-hand portion of the figure. The pass or saddle point corresponds to the critical deformation of unstable equilibrium. To the extent to which we may use classical terms, the course of the fission process may be symbolized by a ball lying in the hollow at the origin of coordinates (spherical form) which receives an impulse (neutron capture) which sets it to executing a complicated Lissajous figure of oscillation about equilibrium. If its energy is sufficient, it will in the course of time happen to move in the proper direction to pass over the saddle point (after which fission will occur), unless it loses its energy (radiation or neutron re-emission). At the right is a cross section taken through the fission barrier, illustrating the calculation in the text of the probability per unit time of fission occurring.

Langevin shape dynamics

- 1) Define a suitable parametrized family of nuclear shapes: $\chi = \{\chi_i\}$
- 2) Calculate the potential energy of deformation: $U(\chi) = U(\{\chi_i\})$
- 3) Calculate the inertial mass tensor: $K(\chi, \dot{\chi}) = \frac{1}{2} \dot{\chi} \cdot M(\chi) \cdot \dot{\chi} = \frac{1}{2} \sum_{ij} \dot{\chi}_i M_{ij}(\chi) \dot{\chi}_j$
- 4) Calculate the friction tensor: $\mathcal{F}(\chi, \dot{\chi}) = \frac{1}{2} \dot{\chi} \cdot \gamma(\chi) \cdot \dot{\chi} = \frac{1}{2} \sum_{ij} \dot{\chi}_i \gamma_{ij}(\chi) \dot{\chi}_j$
- 5) Add the stochastic forces (dissipation => fluctuation):

=> *Langevin equation of motion:*

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\chi}_i} \right) = \frac{\partial \mathcal{L}}{\partial \chi_i} - \frac{\partial \mathcal{F}}{\partial \dot{\chi}_i} + \Gamma_i$$

Kramers, Physica 7 (1940) 284, ...

Abe, Ayik, Reinhard, Suraud, Phys Rep 275 (1996) 49

Fröbrich & Gontchar, Phys Rep 292 (1998) 131

Chadhuri & Pal, Phys Rev C63 (2001) 064603

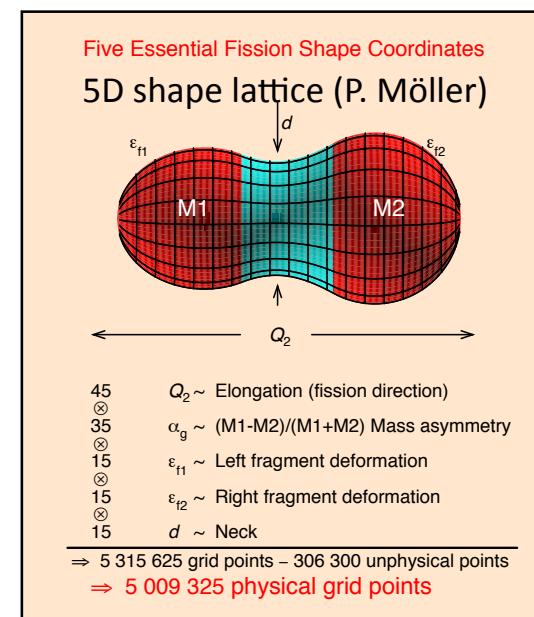
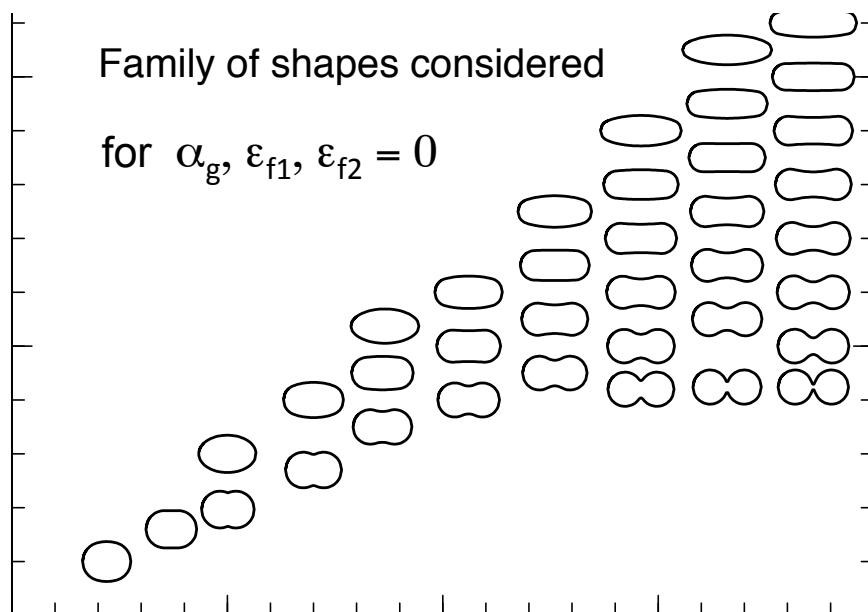
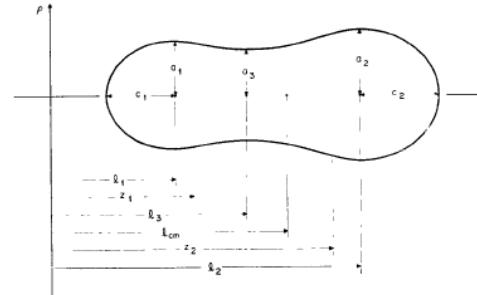
Karpov, Nadtochy, Vanin, Adeev, Phys Rev C63 (2001) 054610

Nadtochy, Kelic, Schmidt, Phys Rev C75 (2007) 0644614

*(This list is
incomplete)*

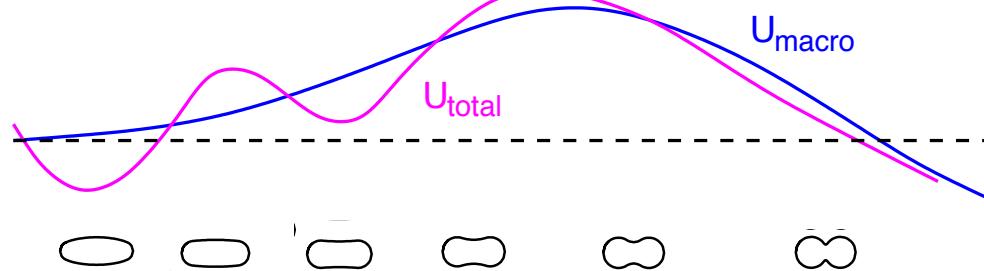
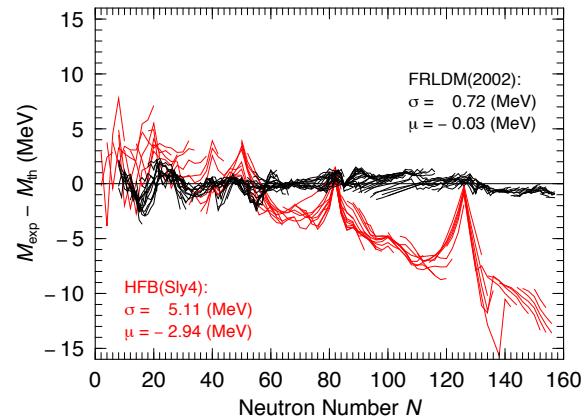
Nuclear shapes relevant for fission

5D shape family:
 3 quadratic surfaces of revolution
 [J.R. Nix, NPA130 (1969) 241]



P. Möller *et al*, Phys Rev C79, 064304 (2009)

Potential energy: *Macroscopic-microscopic method*



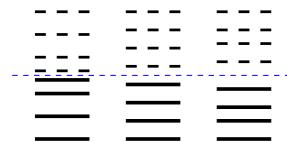
$$E(Z, N, \text{shape}) = E_{\text{macro}}(Z, N, \text{shape}) + E_{\text{micro}}(Z, N, \text{shape})$$

*Finite range
liquid drop*

$$E_{\text{macro}}(Z, N, \chi) = -a_{\text{vol}}(1-\kappa_{\text{vol}}I^2)A - a_{\text{surf}}(1-\kappa_{\text{surf}}I^2)B_1 A^{2/3} + c_1 \frac{Z^2}{A^{1/3}} B_3 + \dots$$

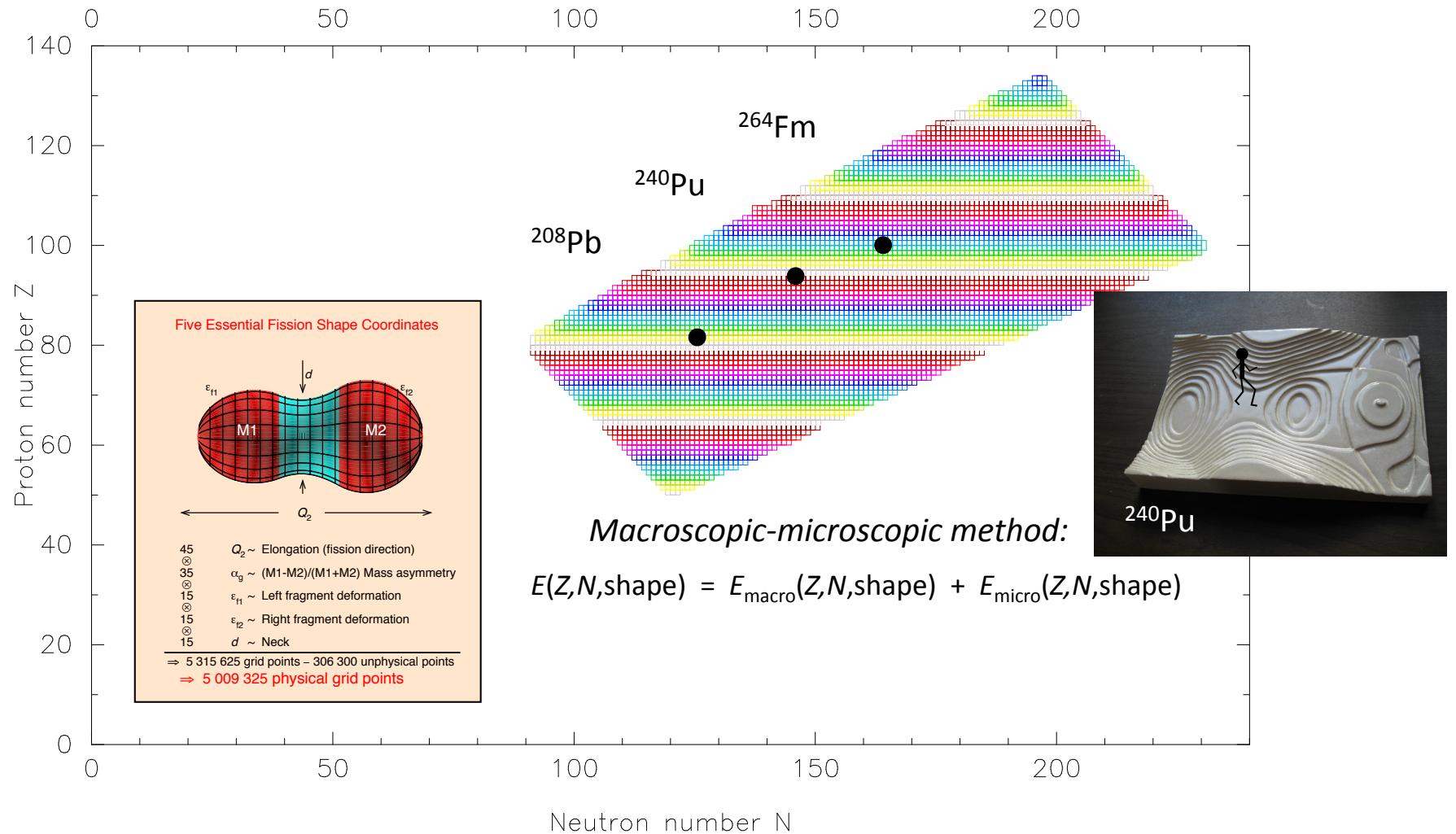
$$E_{\text{micro}}(Z, N, \chi) = E_{\text{shell}}(Z, N, \chi) + E_{\text{pair}}(Z, N, \chi)$$

Strutinsky *BCS*



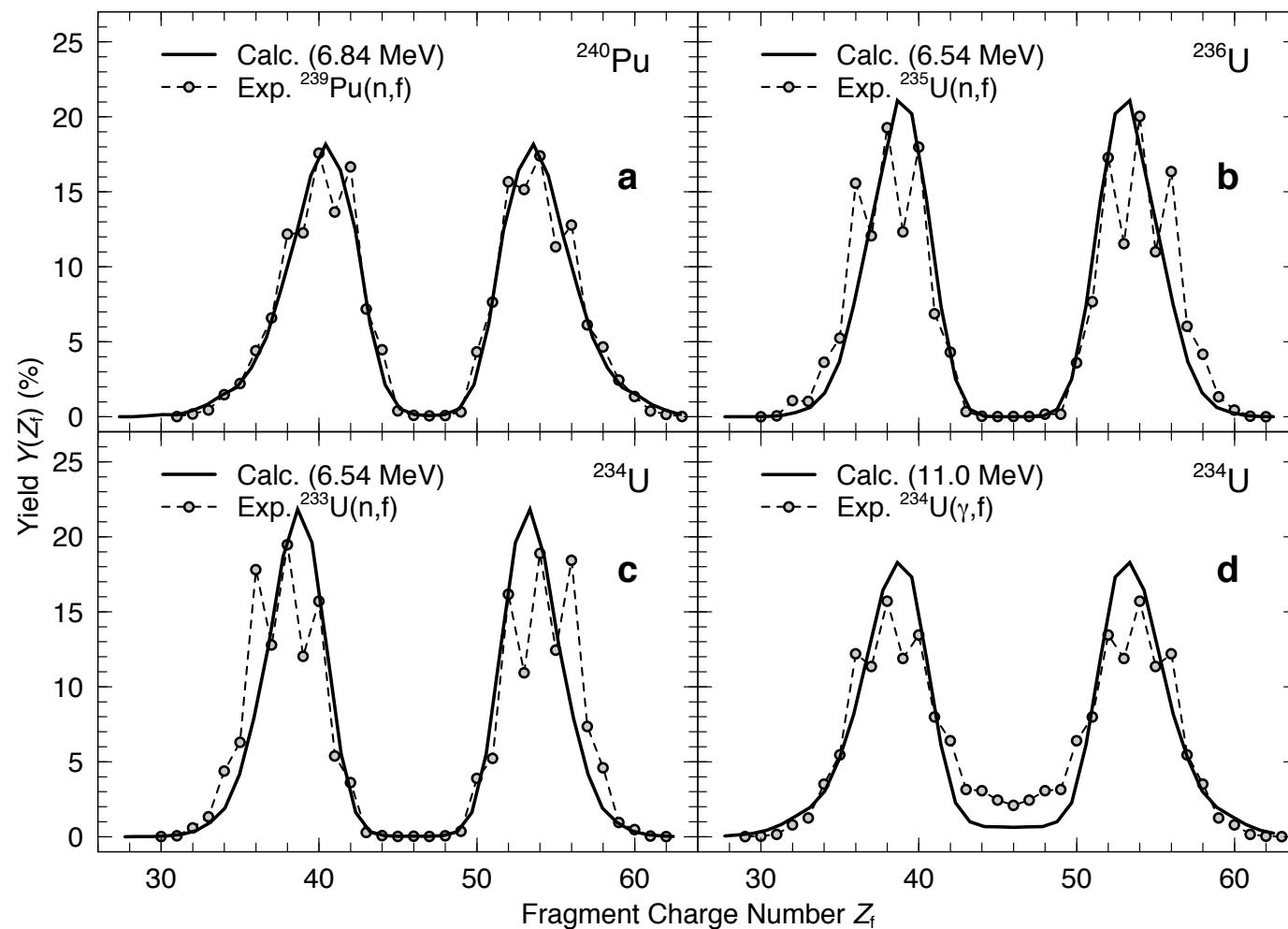
5D deformation-energy surfaces for 5254 nuclei

P. Möller *et al*, Phys Rev C79, 064304 (2009)



$P(A_f)$ from $^{240}\text{Pu}^*$ and $^{236,234}\text{U}^*$

5D Metropolis walks

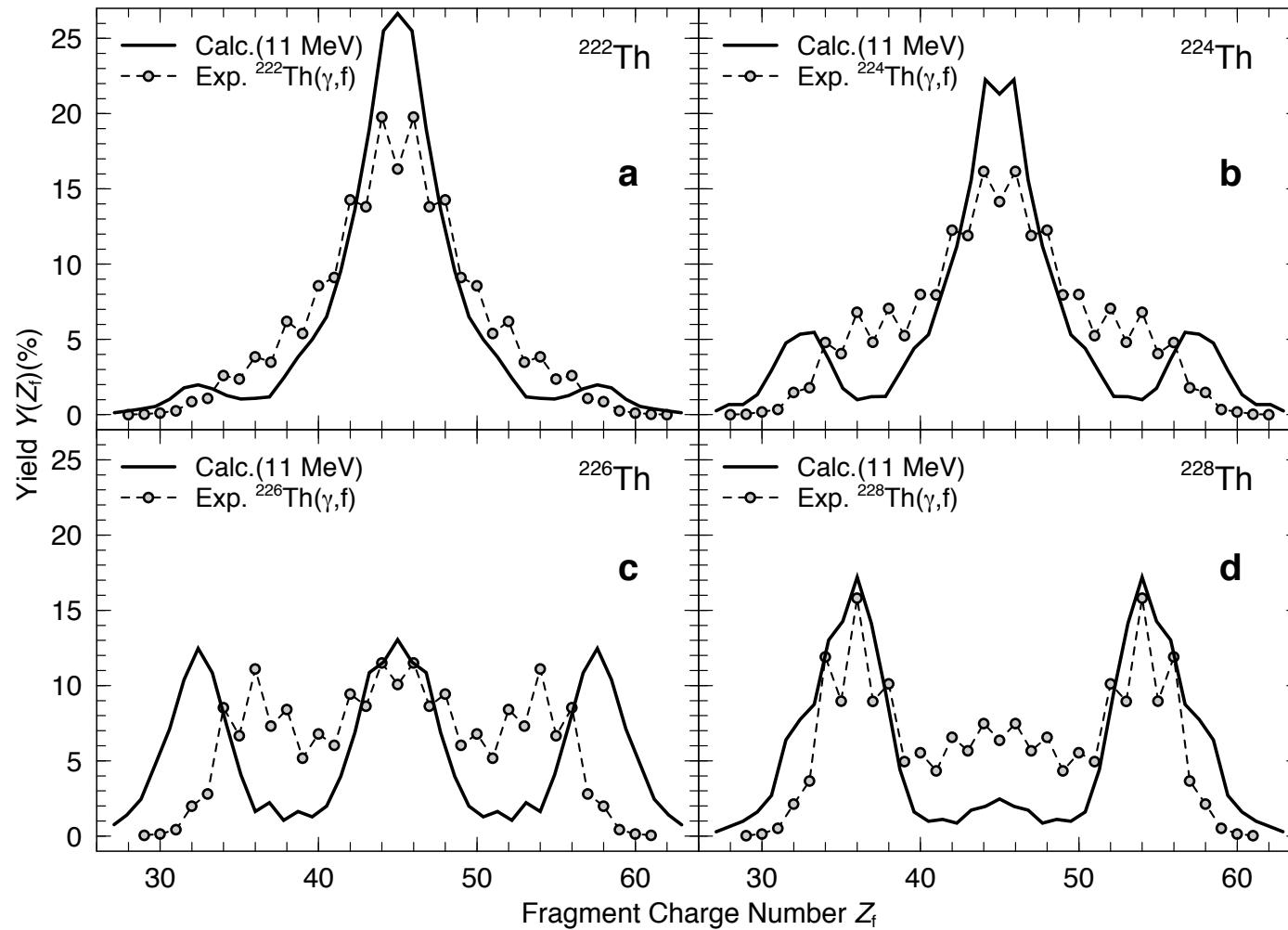


J. Randrup & P. Möller, PRL 106 (2011) 132503

JR: BertschFest 2012

$P(A_f)$ for $^{222,224,226,228}\text{Th}(\gamma,f)$

5D Metropolis walks



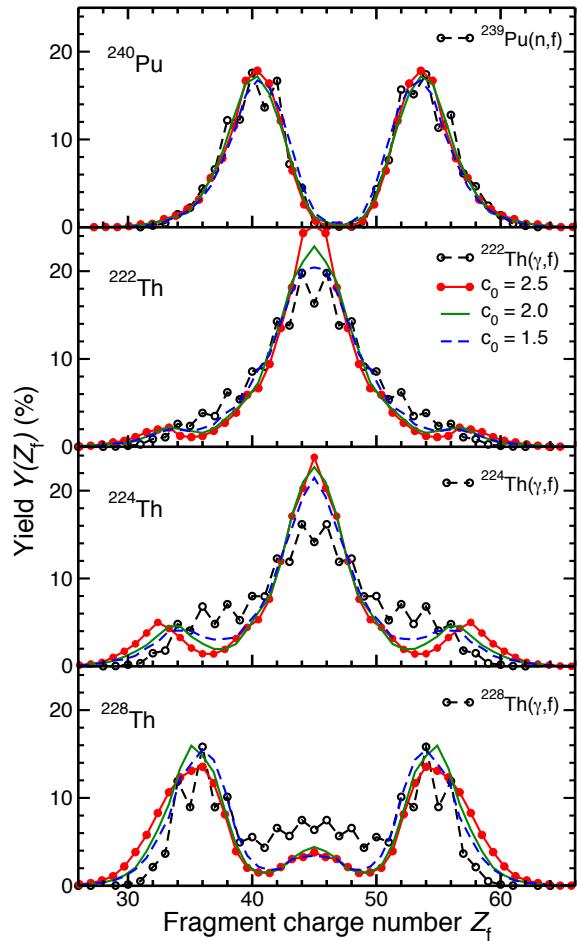
J. Randrup & P. Möller, PRL 106 (2011) 132503

JR: BertschFest 2012

Metropolis walk:

The shape evolves until the neck has shrunk to a specified value c_0

Shape diffusion: robust wrt c_0

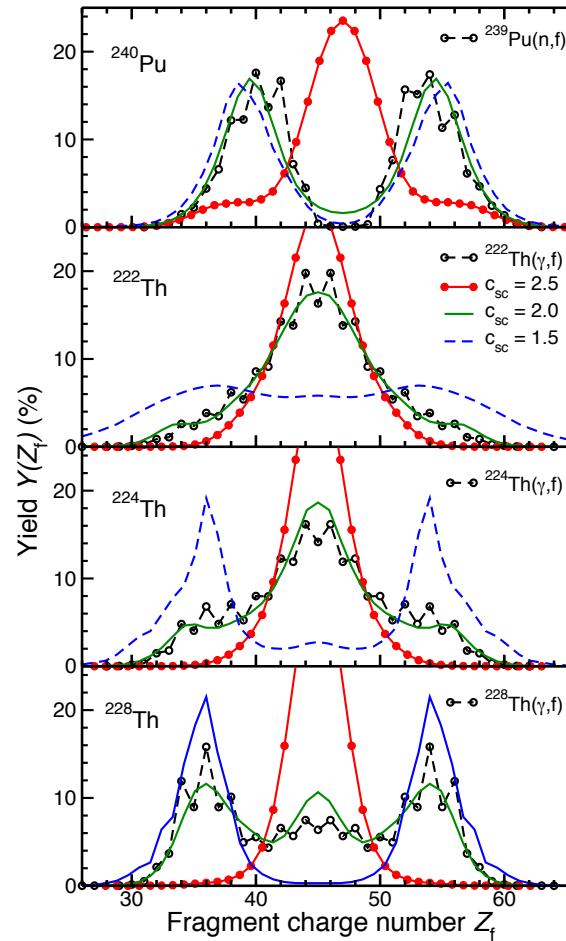


⇒ Shape dynamics on the pre-scission potential landscape is important!

Statistical scission:

Each scission configuration is populated in proportion to its statistical weight*

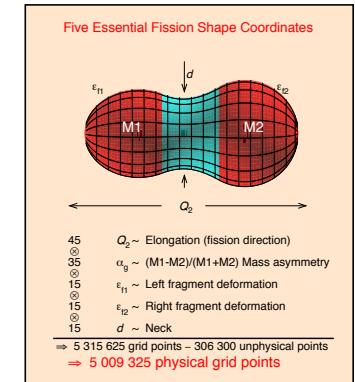
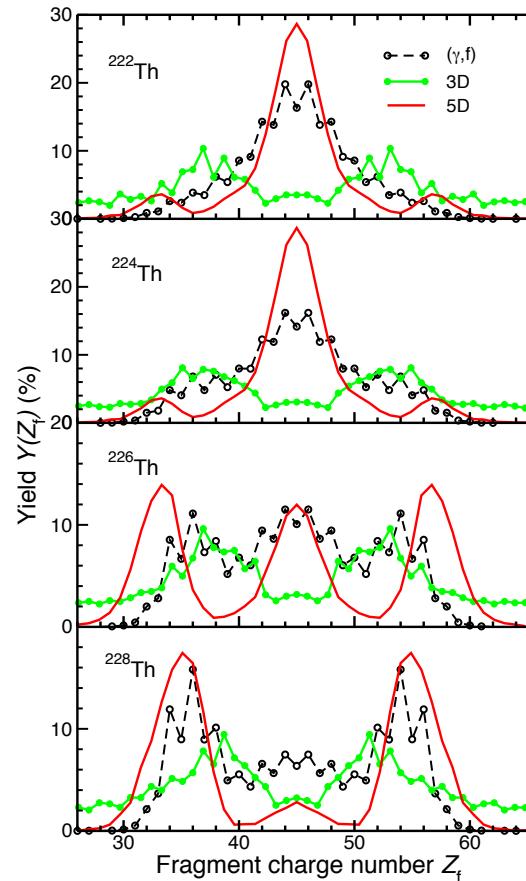
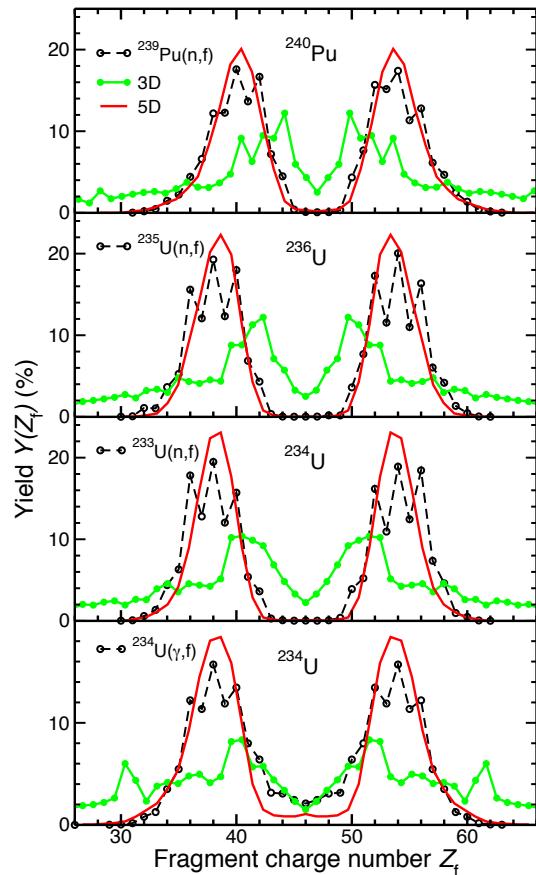
Scission model: sensitive to c_{sc}



* Fong, Phys Rev 102 (1956) 434;
Wilkins et al, PRC 14 (1976) 1832

Restricted shape family?

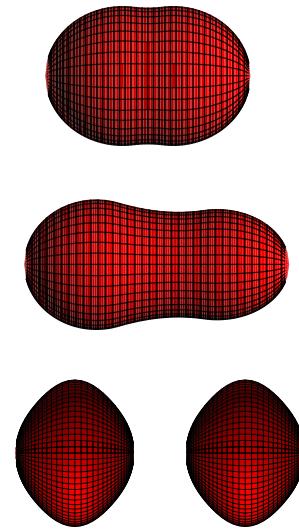
$$5D \rightarrow 3D: V(i,j,m) = \min_{k,l} [V(i,j,k,l,m)]$$



=> Must use sufficiently flexible shapes!

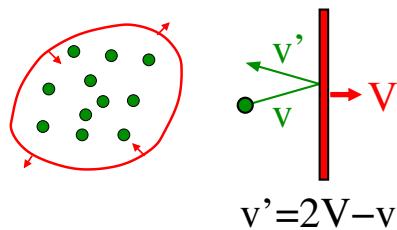
Needed for Langevin shape dynamics:

- ✓ 1) Define a suitable parametrized family of nuclear shapes: $\mathbf{X} = \{X_i\}$
- ✓ 2) Calculate the potential energy of deformation: $U(\mathbf{X}) = U(\{X_i\})$
- 3) Calculate the dissipation tensor $(\mathbf{M}(\mathbf{X}))_{ij}(\mathbf{X})$
- 4) Calculate the dissipation tensor $(\mathbf{M}(\mathbf{X}))_{ij}(\dot{\mathbf{X}})$



Nuclear shape dynamics is highly dissipative

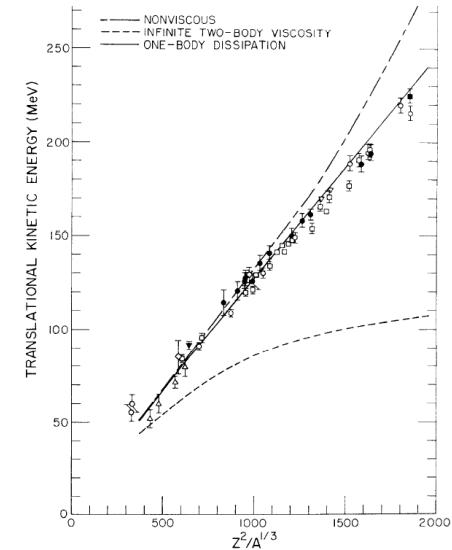
J. Blocki, Y. Boneh, J. R. Nix, J. Randrup, M. Robel, A. J. Sierk, and W. J. Swiatecki,
Ann Phys **113** (1978) 330: One-Body Dissipation and the Super-Viscosity of Nuclei



One-body wall dissipation:

$$\dot{Q} = m\rho_0 \bar{v} \int d^2\sigma \dot{n}^2$$

.. is *strong!*



Strong dissipation => Creeping evolution => Acceleration and (velocity)² are small => Inertial mass is unimportant

Smoluchowski Equation:

$$\mathbf{F}^{\text{pot}} + \mathbf{F}^{\text{fric}} + \mathbf{F}^{\text{ran}} \doteq \mathbf{0}$$

↑ ↓ ↓

driving force dissipative force

$$\left. \begin{array}{l} \mathbf{F}^{\text{pot}} = -\partial U / \partial \chi \\ \mathbf{F}^{\text{fric}} = -\partial \mathcal{F} / \partial \dot{\chi} = -\gamma \cdot \dot{\chi} \\ \langle \mathbf{F}^{\text{ran}}(t) \rangle = \mathbf{0} \\ \langle F_i^{\text{ran}}(t) F_j^{\text{ran}}(t') \rangle = 2T\gamma_{ij}\delta(t-t') \end{array} \right\}$$

Strongly damped nuclear shape dynamics: Brownian motion

Strong dissipation => creeping evolution => mass unimportant

Smoluchowski Equation:

$$\mathbf{F}^{\text{pot}} + \mathbf{F}^{\text{fric}} + \mathbf{F}^{\text{ran}} \doteq \mathbf{0}$$

$$\left\{ \begin{array}{l} \mathbf{F}^{\text{pot}} = -\partial U / \partial \chi \\ \mathbf{F}^{\text{fric}} = -\partial \mathcal{F} / \partial \dot{\chi} = -\boldsymbol{\gamma} \cdot \dot{\chi} \\ \langle \mathbf{F}^{\text{ran}}(t) \rangle = \mathbf{0} \\ \langle F_i^{\text{ran}}(t) F_j^{\text{ran}}(t') \rangle = 2T\gamma_{ij}\delta(t-t') \end{array} \right.$$

Brownian motion

$$\dot{\chi} = \boldsymbol{\mu} \cdot (\mathbf{F}^{\text{pot}} + \mathbf{F}^{\text{ran}})$$

Mobility tensor:

$$\boldsymbol{\mu} \equiv \boldsymbol{\gamma}^{-1} \quad \mu_{ij} = \sum_n \tilde{\chi}_i^{(n)} \tilde{\chi}_j^{(n)}$$

Solve EoM by direct numerical simulation:

$$\delta \chi_i = \sum_n \tilde{\chi}_i^{(n)} \left[\Delta t \tilde{\chi}^{(n)} \cdot \mathbf{F}^{\text{pot}} + \sqrt{2T\Delta t} \xi_n \right]$$

→ *Isotropic mobility* => simple random walk on the lattice => *Metropolis*

Isotropic mobility tensor => Metropolis walk on shape lattice

If μ is diagonal: $\delta\chi_i = \mu_i F_i \Delta t + \sqrt{2T\mu_i \Delta t} \xi_i$

$$\begin{aligned} F_i &= -\partial U(\chi)/\partial \chi_i \\ \mu_i &= 1/\gamma_i \end{aligned}$$

Probability for taking a (forwards or backwards) step during the time Δt :

$$P_i^\pm = \nu_i^\pm \Delta t \quad \nu_i^\pm : \text{Transition rates}$$

Drift coefficient: $\mathcal{V}_i = [\nu_i^+ - \nu_i^-] \Delta_i = \mu_i F_i$

Diff. coefficient: $\mathcal{D}_i = \frac{1}{2}[\nu_i^+ + \nu_i^-] \Delta_i^2 = \mu_i T$

=> Transition rates: $\nu_i^\pm = \frac{\mu_i}{\Delta_i^2} [T \pm \frac{1}{2}F_i \Delta_i] \approx [T \pm \frac{1}{2}\Delta U_i]$

The ratio between the probabilities for stepping forwards or backwards:

$$P_i^+ / P_i^- \approx e^{-\Delta U_i / T}$$

→ Metropolis

Metropolis walk on a lattice: $P(\text{step}) = \begin{cases} \Delta U \leq 0 : 1 \\ \Delta U \geq 0 : \exp(-\Delta U/T) \end{cases}$

Structure of the mobility tensor?

Dissipation rate:
1b wall formula

$$\dot{Q} = m\rho_0 \bar{v} \oint d^2\sigma \dot{n}^2$$

$$\dot{Q} = \sum_{ij} \dot{\chi}_i \gamma_{ij}(\chi) \dot{\chi}_i = \sum_{\mu\nu} \dot{q}_\mu g_{\mu\nu}(q) \dot{q}_\nu$$

Friction tensor in
the Nix variables:

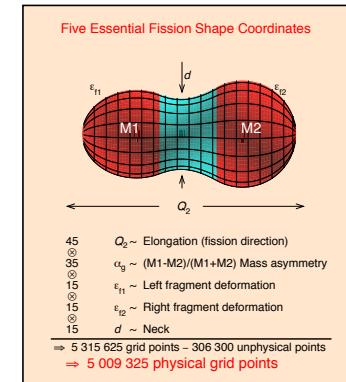
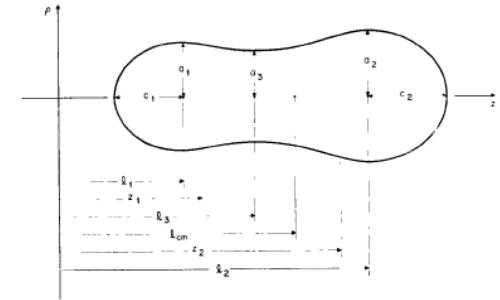
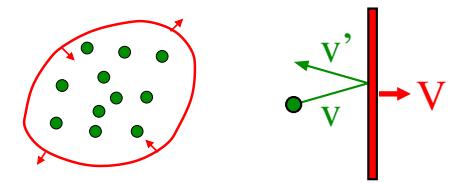
$$g_{\mu\nu} = \frac{\pi}{2} m \rho_0 \bar{v} \int \frac{\partial \rho^2(z)}{\partial q_\mu} \frac{\partial \rho^2(z)}{\partial q_\nu} \left[\rho^2(z) + \frac{1}{4} \left(\frac{\partial \rho^2}{\partial z} \right)^2 \right]^{-\frac{1}{2}} dz$$

Friction tensor γ in
the lattice variables:

$$\gamma_{ij}(\chi) = \sum_{\mu\nu} \frac{\partial q_\mu}{\partial \chi_i} g_{\mu\nu}(q) \frac{\partial q_\nu}{\partial \chi_j}$$

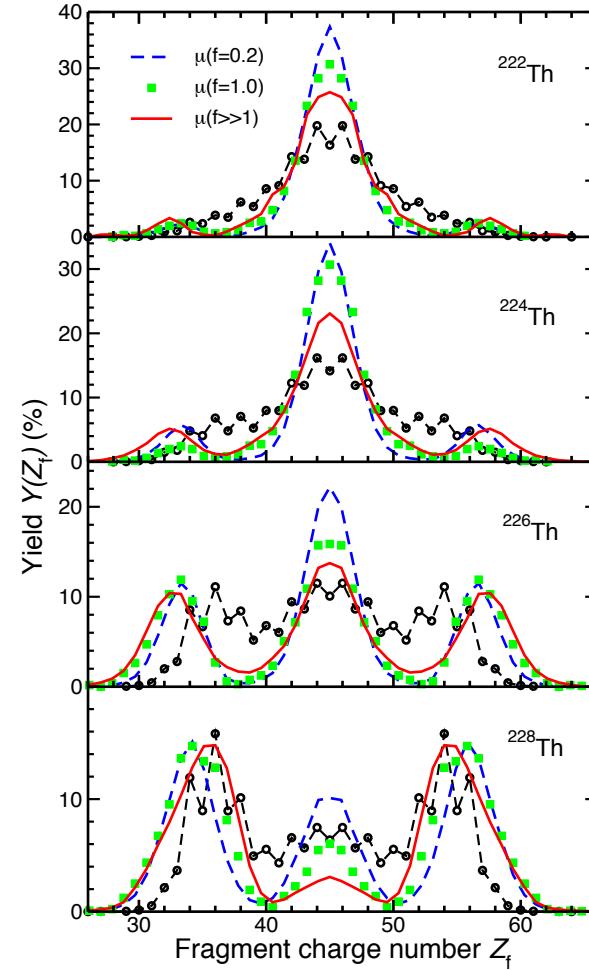
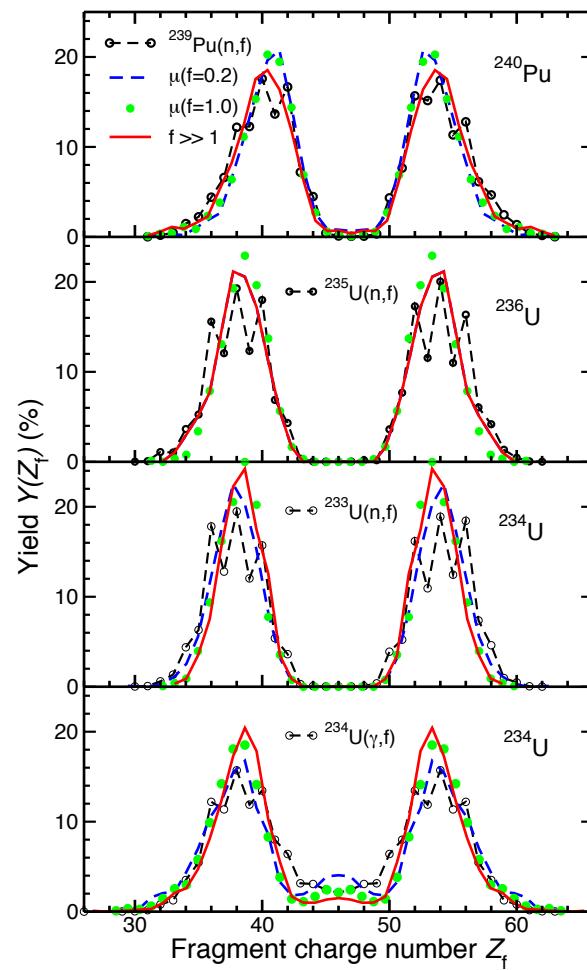
Isotropize γ at
each lattice site:
 $0 \leq f \leq \infty$

$$\tilde{\gamma}(f) : \tilde{\gamma}_n(f) \equiv \frac{\gamma_n + f \bar{\gamma}}{1 + f} \quad \text{where} \quad \bar{\gamma} \equiv \frac{1}{D} \sum_{n=1}^D \gamma_n$$



Dependence of $P(A_f)$ on the mobility tensor

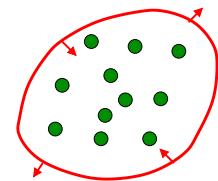
$$\tilde{\gamma}(f) : \quad \tilde{\gamma}_n(f) \equiv \frac{\gamma_n + f\bar{\gamma}}{1+f} \quad \Rightarrow \quad \tilde{\mu}(f) = \tilde{\gamma}(f)^{-1} \quad f = 0.2, 1.0, \infty$$



Main points:

*Shape motion is strongly damped => ignore inertial masses
=> Smoluchowski equation (Brownian motion)*

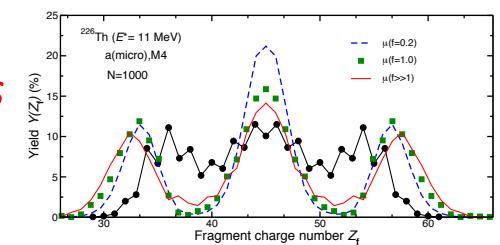
$$\dot{\chi} = \mu \cdot (\mathbf{F}^{\text{pot}} + \mathbf{F}^{\text{ran}})$$



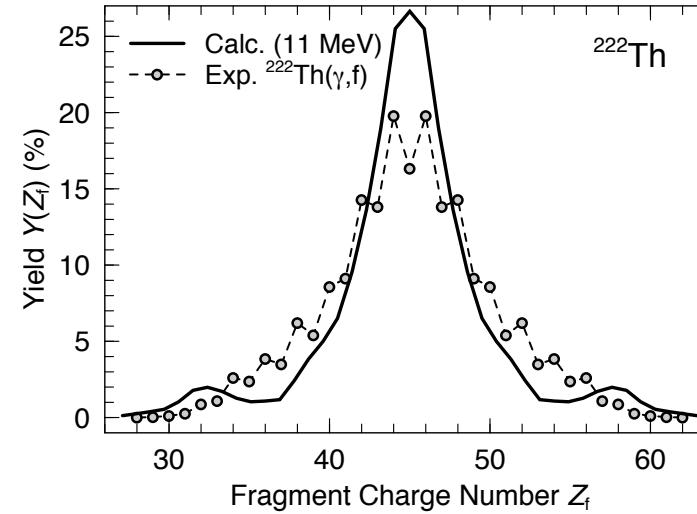
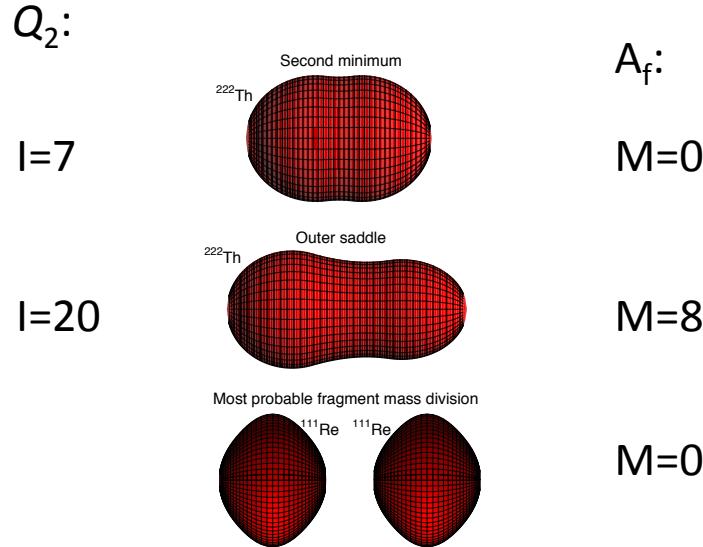
*P(A_f) depends only weakly on the dissipation tensor
=> Metropolis walk is a reasonable starting point*



The dependence on the dissipation anisotropy provides an estimate of the uncertainty on the calculated P(A_f)

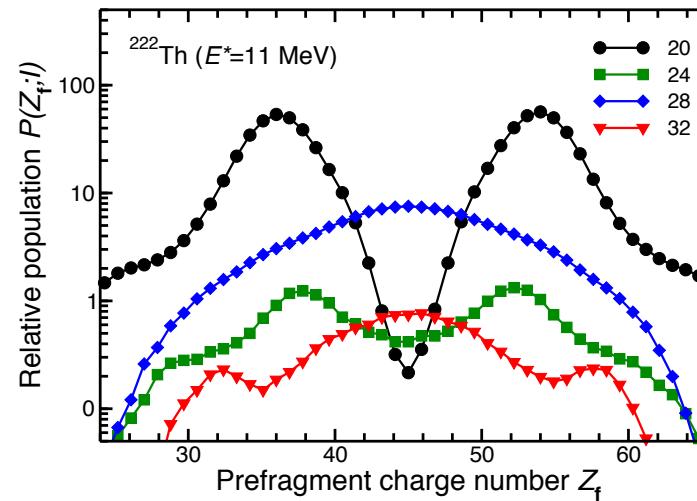


^{222}Th : Mass asymmetry is NOT determined at the saddle!



Distribution of mass asymmetries
at a specified fixed elongation Q_2 :

$$P(A_f; Q_2) \sim \sum_n \delta(I_n - I) \delta(M_n - M) \gamma$$

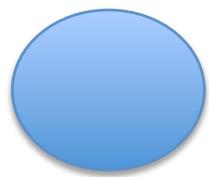


^{226}Th : Shape dependence of the Wigner term?

$$E(Z, N, \text{shape}) = E_{\text{macro}}(Z, N, \text{shape}) + E_{\text{micro}}(Z, N, \text{shape})$$

$$E_{\text{macro}}(Z, N, \text{shape}) = \dots + W(\text{shape}) \frac{|N - Z|}{A}$$

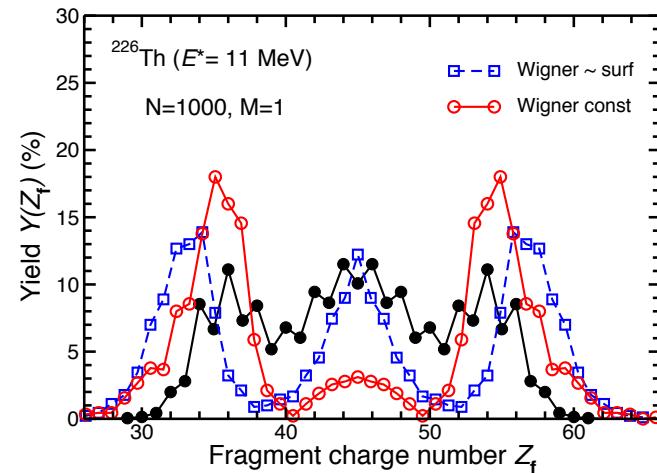
One nucleus



Two nuclei



$$W(\bullet \bullet) = W(\bullet) + W(\bullet)$$



⇒ The shape dependence
of the Wigner term
influences $P(A_f)$

⇒ The mass distribution
is sensitive to details
of the energy surface



Summary and perspectives

Novel method for calculating fission fragment mass distributions

Augments the standard compound nucleus picture
with explicit simulation of the equilibration *dynamics*

- Required:
- The deformation-energy landscape for a *sufficiently rich* family of fission shapes
 - The friction tensor for the shape motion
 - Unprecedented *predictive power*
 - Requires only relatively *modest* computing power
 - Preliminary application possible to >5,000 nuclei
for which the 5D surfaces are already available
 - A number of model aspects need further study
 - Extensions anticipated
- Conceptually very simple
- Very important
- Less crucial
- Useful tool
- ~500,000 hours vs
~min on a laptop
- Light Hg region;
end of the *r*-process?
- Friction tensor;
energy dep; inertias
- Spontaneous fission?
Fragment TKE?

